Diagrammatic Monte Carlo simulations of the Ising and $\Phi^4$ models

Lode Pollet

collaborators:

Nikolay Prokof’ev and Boris Svistunov

Tobias Pfeffer

previous/other collaborators: J. Gukelberger, E. Gull, E. Kozik, P. Kroiss, S. Schultess, M. Troyer, K. Van Houcke, F. Werner
Perturbative expansions

\[ H = H_a + H_b \]

Continuous time

\[ Z = \text{Tr} T_\tau e^{-\beta H_a} \exp \left[ - \int_0^\beta d\tau H_b(\tau) \right] \]
\[ = \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)]. \]

Strong coupling expansions:
- Two-body term is $H_a$; choose basis where this is diagonal
- Typically on finite system (requires finite size analysis), finite $\beta$
- Can be sign-free for bosons; spins with AF couplings on bipartite lattices, ...

Weak coupling expansions:
- One-body term is $H_a$; typically thermodynamic limit, can be ground state. Has Wick theorem, Dyson equation, etc

Not talking about variational Monte Carlo, diffusion Monte Carlo, auxiliary field...
Diagrammatic expansions

\[ F(y) = \sum_{n} \sum_{x_1, \ldots, x_n} D(x_1, \ldots, x_n; y) \]

main idea: sample over all expansion orders \( n \) and all different topologies \( D \) (involves transitions between the same and different expansion orders)

internal variables \( \{x\} \) while \( y \) is an external variable
some of the \( \{x\} \) could be continuous variables in which case differentials matter
I. Review

- impurity models:
  - Frohlich, acoustic phonon, BEC impurity, SSH model, many-polaron
  - *Fermi polaron* (3d, 2d, mass imbalance, ...)
  - out of equilibrium: relaxation of current through a quantum dot

- **Hubbard model**:
  - Fermi liquid regime
  - spin-dependent hopping as a model for Bose liquid?
  - FFLO
  - pairing(s,p,d,...) instabilities for weak interactions

- **resonant fermions**
  - fermionic quantum simulator

- **frustrated magnetism**
  - Heisenberg model on triangular lattice

- algorithmic developments
  - skeleton diagrams (first illustrated for scattering problem); partial resummations
  - convergence issues
  - Popov-Fedotov and fermionization
  - (non)-existence of Luttinger-Ward functional
  - combination with DCA/DMFT?
Frohlich polaron

\[ H_{e-ph} = \sum_{k,q} V(q)(b_q^\dagger - b_{-q})a_{k-q}^\dagger a_k \]

\[ V(q) = i(2\sqrt{2}\alpha\pi)^{1/2} \frac{1}{q} \]

\[ D(q, \tau_2 - \tau_1) = \exp[-\omega_p(\tau_2 - \tau_1)] \]

\[ \tilde{D}(q, \tau_2 - \tau_1) = |V(q)|^2 \exp[-\omega_p(\tau_2 - \tau_1)] \]

essentially a single particle coupled to a bosonic bath

typical diagrammatic structure for G:

this is a sign positive expansion!!

Frohlich polaron

note the local character of the update
Frohlich polaron

Similar methods: acoustic polaron and Bose polaron (impurity in a BEC)

First results for Hubbard (~2009)

diagrammatic Monte Carlo: $U/t=4$; Fermi-liquid regime; 2d and 3d

$$\Sigma = G_{\uparrow} + \Sigma_{\text{tadpoles absorbed in bare Green functions}} + \Sigma_{\text{DMFT}} + \ldots$$

DCA (dynamical cluster approximation) and its lowest order DMFT (dynamical mean-field theory) allow for an unbiased answer when extrapolated in the cluster size -- see later

Fermi polaron

\[ |\psi\rangle = \phi_0 |\text{GS}\rangle + \sum_{k,q} \phi_{k,q} |k, q\rangle \]

where \( q < k_F; k > k_F \)


F. CHEVY PHYSICAL REVIEW A 74, 063628 (2006)
<table>
<thead>
<tr>
<th>$N$</th>
<th>$\text{Bare}$</th>
<th>$\text{Bold } G$</th>
<th>$\text{Bold } G-G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>34</td>
<td>34</td>
<td>13</td>
</tr>
<tr>
<td>6</td>
<td>210</td>
<td>206</td>
<td>74</td>
</tr>
<tr>
<td>7</td>
<td>1,526</td>
<td>1,476</td>
<td>544</td>
</tr>
<tr>
<td>8</td>
<td>12,558</td>
<td>12,123</td>
<td>4,458</td>
</tr>
<tr>
<td>9</td>
<td>115,618</td>
<td>111,866</td>
<td>41,221</td>
</tr>
<tr>
<td>10</td>
<td>1,177,170</td>
<td>1,143,554</td>
<td>421,412</td>
</tr>
<tr>
<td>11</td>
<td>13,136,102</td>
<td>12,816,572</td>
<td>4,722,881</td>
</tr>
<tr>
<td>12</td>
<td>159,467,022</td>
<td>156,217,782</td>
<td>57,553,440</td>
</tr>
</tbody>
</table>
\[ k_F a = 0.75 \]
(quasi)-2d:

\[ \text{polaron-molecule transition in agreement with variational 2ph polaron energy calculation} \]


Mass imbalance (3d):


not fully understood what is going on

simple analytical structure of the polaronic ground state:

(essentially Landau’s argument for the validity of Fermi liquid theory)


FIG. 1. Examples of (top) “exchange-hole” and (bottom) “direct-hole” contributions to the 2-ph diagrams are shown. This demonstrates that every order \( N > 2 \) has at least two diagrams counting as 2-ph.
5 Hédin equations:

\[
\begin{align*}
G & = G_0 + G_0 \Sigma \\
\Sigma & = i \Gamma W \\
\Pi & = -2i \Gamma G \\
\Gamma & = I + \Gamma W + \ldots
\end{align*}
\]

Dyson equation for propagator
irreducible selfenergy
effective potential
irreducible polarization
irreducible vertex

functional derivate makes the set of equations closed

L. Hedin. Phys. Rev. 139, A796 (1965)
do skeleton series make sense?

**NO!**

- Diverge for large $g$, even if convergent for small $g$.
- Dyson collapse: series is asymptotic if for some (e.g., complex) $g$ one finds pathological behavior.
- QED: $e \rightarrow ie$.
- Bosons: collapse for negative $U$.
- Anharmonic oscillator.

**YES / PERHAPS!**

- Dyson’s collapse argument does not hold for lattice Fermi-model at finite temperature.
- Not known whether it applies to skeleton diagrams.
- There exist regularization schemes.
- Due to “sign blessing” orders may compensate each other leading to a finite convergence radius.

- Pollet, Prokofev, Svistunov, PRL 2010
- Turn anharmonic oscillator into something with infinite convergence radius.

- Even nr of skeleton diagrams grows factorially (zero convergence radius).
- Molinari et al.
resonant fermions

Controllable results for resonant fermions promoting the system to the major testing ground for theories of strongly correlated fermions.

Unprecedented experimental precision in the field of ultra-cold atoms

Virial expansion (first 3 terms)

\[ G = G^0 + G^0 \Sigma G \]
\[ \Gamma = \Gamma^0 + \Gamma^0 \Pi \Gamma \]
\[ \Sigma = \Gamma + \Gamma^0 + \ldots \]
\[ \Pi = G G^0 G^0 G + \ldots \]

Frustrated magnetism

Consider the Heisenberg model on a triangular lattice:

$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

express in terms of fermions:

$$\vec{S}_i = \frac{1}{2} \sum_{\alpha, \beta} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha, \beta} c_{i, \beta}$$

flat band!

Popov-Fedotov trick: project out unphysical configurations with 0 or 2 fermions to arrive at diagrammatic technique,

$$H_F \to H_F - i \frac{\pi}{2} T \sum_i (n_i - 1)$$
Frustrated magnetism

uniform susceptibility and compared with linked-cluster expansion
calculation limited by development of near singularity at $Q = (4\pi/3, 0)$

Weak coupling instabilities of the 2d Hubbard model

See talk by Boris Svistunov later this week

Youjin Deng, Evgeny Kozik, Nikolay V. Prokof'ev, Boris V. Svistunov, EPL 110 (2015) 57001
Weak coupling phase diagram of an attractive 2d Hubbard model with spin-dependent hopping

attractive 2d Hubbard model with mass imbalance

is combining DMFT + diagrammatic Monte Carlo possible?

Adv: some ideas about error bars possible

test model: Anderson localization, gaussian disorder

\[ H = -J \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i \epsilon_i \hat{n}_i \]

Vertex corrections will be a real challenge

however: non-existence of unique Luttinger-Ward functional and misleading convergence:


further refinements: Riccardo Rossi, Felix Werner, Nikolay Prokof’ev, Boris Svistunov arXiv:1508.03654

dangers of partial resummation for Hubbard models:

Numerically Exact Long Time Behavior of Nonequilibrium Quantum Impurity Models

Emanuel Gull,1 David R. Reichman,2 and Andrew J. Millis1

1Department of Physics, Columbia University, New York, New York 10027, USA
2Department of Chemistry, Columbia University, New York, New York 10027, USA

(Dated: May 9, 2011)

\[ H_A = \sum_{\sigma} (\varepsilon_d + H\sigma) \, d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow + H_{hyb} + H_{lead} \]

with NCA resummation: very long times accessible; also Kondo regime should be accessible; in principle not more difficult than the Fermi-polaron problem.
Diagrammatic Monte Carlo

+ • frustrated magnets: better than series expansions
  • Hubbard models (instabilities, FFLO and spin-dependent hopping): better than determinant QMC
  • resonant fermions: nothing else

main potential: it is fun to do (and find out) what nobody else can do
  • long-range interactions, screening
  • out-of-equilibrium (Keldysh formalism)
  • gauge theories? lattice QCD?
  • universal parlance, thermodynamic system, real frequencies, (partial) resummations can be exploited, ...

− • usually a (hidden) simplifying factor when it works; ie with competing instabilities we have difficulties
  • series convergence issues; only low orders can be reached; extrapolations can easily be uncontrolled
  • technical issues: storage of vertex etc
  • we lack manpower, and it is highly technical work of the high-risk high-gain caliber which is not suited for everyone
II. Bi-grassmanns for bond models

**bond:**

- can have different modes $\alpha_b$
- with weights $f(\alpha_b)$
- ground state $f(0) = 1$
- each mode can be occupied or not

This hardcore bosonic constraint is mapped on two pairs of conjugate grassmannian variables:

$$A_b = \exp \left( \sum_{\alpha \neq 0} \bar{\xi}_\alpha \xi_\alpha + \frac{1}{f(\alpha)} \bar{\xi}_\alpha \xi_\alpha \right)$$

$$= \prod_{\alpha \neq 0} e^{\bar{\xi}_\alpha \xi_\alpha} e^{\frac{1}{f(\alpha)} \bar{\xi}_\alpha \xi_\alpha}.$$

Site factors must be uniquely determined by the adjacent bond occupations:

$$B_j = \sum_{\{\alpha_b\}_j} g(\{\alpha_b\}_j) \prod_{b \in \{b\}_j} \bar{\xi}_{\alpha_b} \xi_{\alpha_b}^*$$

$$= 1 + \sum_{\{\alpha_b\}_j \neq 0} g(\{\alpha_b\}_j) \prod_{b \in \{b\}_j} \bar{\xi}_{\alpha_b} \xi_{\alpha_b}^*.$$
Application: 2d Ising model (I know it is exactly solvable)

Hamiltonian:

\[-H/T = \beta \sum_{\langle i,j \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i.\]

Partition function:

\[Z = \sum_{\{\sigma_i\}} \prod_{\langle i,j \rangle} e^{\beta \sigma_i \sigma_j} e^{h \sigma_i}.\]

Spin correlation function

\[\rho_{ij} = \langle \sigma_i \sigma_j \rangle = \frac{1}{Z} \left. \frac{\partial^2 \tilde{Z}}{\partial h_i \partial h_j} \right|_{h_i = h_j = h} \]

Using identities

\[e^{\beta \sigma_i \sigma_j} = \cosh \beta \left( 1 + \sigma_i \sigma_j \tanh \beta \right)\]

\[e^{h \sigma_i} = \cosh h \left( 1 + \sigma_i \tanh h \right)\]

we can write

\[Z = Z_{\text{const}} Z' \quad Z_{\text{const}} = (\cosh \beta)^2 N (\cosh h)^N \quad \zeta = \tanh \beta\]

\[Z' = \sum_{\{\sigma_i\}} \prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j \zeta)(1 + \sigma_i \eta). \quad \eta = \tanh h\]

This is a bond model with bond occupation numbers 0 and 1 and respective weights 1 and \(\zeta\). From now on we set \(\eta = 0\). The site factors also drop out.

do not be misled by the similarity to the high-temperature series expansion; this one here is quite different

PS: this is NOT the exact solution where the domain walls are mapped to non-interacting Grassmann variables (see eg many-body lecture notes by C. Nayak)
Vertex building blocks:

\[ Z' = \prod_b \int \mathcal{D}[\ldots]_b \exp \left( \xi_b^\dagger \xi_b + \frac{1}{\zeta} \xi_b^\dagger \xi_b \right) \times \exp \left( \sum_j V_2^j - 2V_4^j \right) \]

(lines 2 and 4 are generic interaction vertices; lines 1 and 3 are the end points for the spin correlation function)

\[ Z' = Z_0 \left( \sum_{n=0}^{\infty} \sum_{x_1,\ldots,x_n} \frac{(-1)^n}{n!} \langle V(x_1) \ldots V(x_n) \rangle_0 \right) \]
Spin correlation function

Along the axes and the diagonal the answer is known analytically:

\[
\rho_{(1,0)} = \coth(2\beta) \left[ \frac{1}{2} + \frac{\cosh^2 2\beta}{\pi} (2 \tanh^2 2\beta - 1) K(k_>) \right] \\
\rightarrow \zeta + 2\zeta^3 + 4\zeta^5 + 12\zeta^7 + 42\zeta^9 + \ldots \\
\rho_{(1,1)} = \frac{2}{\pi k_>} \left[ K(k_>) + (k_>^2 - 1) K(k_>) \right] \\
\rightarrow 2\zeta^2 + 4\zeta^4 + 10\zeta^6 + 32\zeta^8 + 118\zeta^{10} + \ldots
\]

Expansions also exist for general matrix elements of the spin correlation function.

only first order diagram

only two 3rd order diagrams
Spin correlation function

first instance of type-3 vertices
Spin correlation function

disconnected diagram

first instances of fermionic exchanges (minus signs!)
the sum of these 4 diagrams yields -1

symmetry factors occur starting in order 6
susceptibility:

\[ \beta^{-1} \chi = 1 + 4 \zeta + 12 \zeta^2 + 36 \zeta^3 + 100 \zeta^4 + 276 \zeta^5 + 740 \zeta^6 + 1972 \zeta^7 + 5172 \zeta^8 + 13492 \zeta^9 + 34876 \zeta^{10} + 89764 \zeta^{11} + 229618 \zeta^{12} + 585508 \zeta^{13} + 1486308 \zeta^{14} + \ldots \]

Table I. Coefficients in the high-temperature series expansion for the correlation function up to order 11.
can we understand the transition from a simpler diagrammatic structure?

G^2W skeleton expansion:

\[ \Pi_{\text{irr}} = \frac{V_2}{1 - V_2 \Pi_{\text{irr}}} \]

\[ \Sigma = \frac{\Pi_{\text{irr}}}{1 - V_2 \Pi_{\text{irr}}} \]

\[ W = V_2 + V_2 \Pi_{\text{irr}} W \]

\[ G = G_0 + G_0 \Sigma G \]

how well does this pole describe the transition?

note: G remains local; all quantities are tensors
1d case:

There is only one type of interaction vertices:

so: no loops, no backtracking, no minus signs

the 0th order in the \( G^2W \) scheme solves the problem exactly:

\[
\begin{align*}
\Pi_{\text{irr}} &= \Pi_0 = \zeta \\
\Sigma &= 0 \\
G &= G_0 \\
W &= \frac{V}{1 - V\Pi_{\text{irr}}} = \frac{1}{1 - \zeta}
\end{align*}
\]

we can get the susceptibility as

\[
T\chi = 1 + 2(\zeta + \zeta^2 + \zeta^3 + \ldots) = 1 + 2\frac{\zeta}{1 - \zeta}
\]

with limiting behavior \( \chi \propto \frac{1}{\beta} \exp(2\beta) \) when \( T \rightarrow 0 \).

2d case:

for \( \Pi_{\text{irr}} = \Pi_0 \) pole is found for \( \zeta_c = 1/3 \)

\[
\begin{align*}
\Sigma &= 0
\end{align*}
\]

(work in progress)
III. Homotopy analysis method

(Tobias Pfeffer)

$$Z[J] = \int D[\Phi] e^{-S_E[\Phi]} + \int dx J\Phi$$

$$S_E[\Phi] = \int dx \left( \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{m^2}{2} \Phi^2 + \frac{g}{4!} \Phi^4 \right)$$

$$G(x-y) = \langle \Phi(x)\Phi(y) \rangle$$

$$G^4(x_1, x_2, x_3, x_4) = \langle \Phi(x_1)\Phi(x_2)\Phi(x_3)\Phi(x_4) \rangle$$

$$\Gamma(x_1, x_2, x_3, x_4) = \int_{5,6,7,8} G^{-1}_{1,5} G^{-1}_{2,6} G^{-1}_{3,7} G^{-1}_{4,8} G^4(x_5, x_6, x_7, x_8)$$

From Wilsons RG analysis:

$$\phi^n, n > 4 : \text{ irrelevant operator}$$

$$g^R_6 = \Gamma^6(0, 0, 0, 0, 0, 0) \to 0 \quad \text{for } m_R \to 0$$

iterating to solving non-linear self-consistency equations has usually poor convergence properties

More stable approach: Root finding

$$f(\kappa_2) - \kappa_2 = 0$$

E.g. Newton-Raphson:

$$\kappa_2^{i+1} = \kappa_2^i + \frac{F(\kappa_2^i)}{F'(\kappa_2^i)} \quad \text{our F is of course complicated...}$$

storage of multi-legged objects out of the question
Is it possible to find the root without knowing the intermediate steps?

Yes: Rebuild the root finding. E.g.

\[ \kappa_{i+1}^4 = \kappa_i^4 + \frac{F(\kappa_i^4)}{F'(\kappa_i^4)} = \]
\[ = \frac{\kappa_i^{i-1} + F'(\kappa_i^{i-1})}{F'(\kappa_i^{i-1})} + \frac{F(\kappa_i^{i-1})}{F'(\kappa_i^{i-1})} = \]
\[ = \ldots \]

**Homotopy.** \( f, g \) continuous operators between topological spaces \( X, Y \).
A continuous operator \( H : X \times [0, 1] \rightarrow Y \) is called a homotopy
if \( H(x, 0) = f(x) \) and \( H(x, 1) = g(x) \).

\[ \mathcal{H}[\phi(x, q)] = (1 - q)\mathcal{L}[\phi(x, q) - u_0(x)] + qH(x)\mathcal{N}[\phi(x, q)] = 0 \]

expansion: \( \phi(x, q) = \sum_{m=0}^{\infty} u_m q^m \)

set of equations \( \left. \frac{d^m}{dq^m} \mathcal{H}[\phi(x, q)] \right|_{q=0} = 0 \) m-th order deformation equation
Example: \( \mathcal{N}[\phi(x)] = \phi(x) - g(x) - \int_a^b dt \ K(x, t) f(\phi(t)) \)

\[
\phi(x) = \sum_{m=0}^{\infty} u_m \\
u_m(x) = \frac{1}{(m-1)!} \int_a^b dt \ K(x, t) \sum_{k=1}^{m-1} f^{(k)}(u_0(t)) B_{m-1,k}(1!u_1(t), \ldots, (m-k)!u_{m-k}(t))
\]

Bell Polynomial: combinatorial factor of \( \frac{d^{m-1}}{dq^{m-1}} \)

do the expansion by Monte Carlo sampling (has sign)

current status:

(T. Pfeffer)
Summary

• review: there are now about 5-10 non-trivial examples where diagMC has gone beyond the state of the art

• bi-grassmann description for classical bond models

• can be extended to 3d Ising, frustrated Ising, plaquette models, …

• useful for gauge theories?

• HAM: alternative way of solving selfconsistency equations with perhaps better convergence properties
Gaussian Model $g=0$

Phi4 Classical Worm $g=10$

Phi4 DSE+HAM $g=10$

$G(|i-j|)$

The graph shows the function $G(|i-j|)$ plotted against $|i-j|$ for different models:

- **Gaussian Model $g=0$**
- **Phi4 Classical Worm $g=10$**
- **Phi4 DSE+HAM $g=10$**
$G(k_x, 0)$ diagMC

$G(k_x, 0)$ classical Worm